

Mesoscopic Structures Reveal the Network Between the Layers of Multiplex Datasets

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Multiplex networks describe a large variety of complex systems, whose elements (nodes) can be connected by different types of interactions forming different layers (networks) of the multiplex. Multiplex networks include social networks, transportation networks or biological networks in the cell or in the brain. Extracting relevant information from these networks is of crucial importance for solving challenging inference problems and for characterizing the multiplex networks microscopic and mesoscopic structure. Here we propose an information theory method to extract the network between the layers of multiplex datasets, forming a “network of networks”. We build an indicator function, based on the entropy of network ensembles, to characterize the mesoscopic similarities between the layers of a multiplex network and we use clustering techniques to characterize the communities present in this network of networks. We apply the proposed method to study the Multiplex Collaboration Network formed by scientists collaborating on different subjects and publishing in the American Physical Society (APS) journals. The analysis of this dataset reveals the interplay between the collaboration networks and the organization of knowledge in physics.

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I. INTRODUCTION

Multiplex networks [1, 2] describe a large number of complex systems where the interactions are of different nature. They are formed by a set of N nodes interacting through M different layers (networks). Recently, multiplex networks have been used to characterize a large variety of systems, including social networks [3], transportation network [4], collaboration networks [5, 6], and brain networks [7]. Extracting relevant information from multiplex networks is central for characterizing their microscopic and mesoscopic structure [8–10], for solving challenging inference problems, and for devising good centrality measures [11–13].

Structural correlations are ubiquitous in multilayer networks and can be a powerful tool to extract information from them. For example the overlap of the links [14] in the different layers of multiplex networks has been observed in systems as different as in-silico societies [3], multilayer airport networks [4] or citation-collaboration networks [5]. Moreover it was recently shown [5] that using the information on the link overlap it is possible to extract information that cannot be extracted if the single layers are taken in isolation. Other examples of correlations encoded in multiplex network structures include correlation between the degrees of the same node in different layers [15], and the activity distribution of the nodes [6, 16].

All these structural correlations reflect local properties of multiplex networks. Nevertheless, in complex networks, significant information is encoded in their mesoscale structure, i.e. their organization into several clusters or communities [17, 18].

Recently new modularity measures for multilayer networks [8] have been proposed and new multiplex community detection algorithms have been formulated [19] based on methods devised for single networks [17]. Al-

ternatively inference methods have been proposed to decompose a single network in different layers with distinct community structure [20] or to visualize multiplex networks [21]. Moreover it has been recently observed that the communities on different layers of a multiplex networks typically overlap among each others, forming mesoscale structures that span across different layers. This phenomenon is central for generalizing the concept of community to multilayer networks [8, 19] and modeling the emergence of communities [22].

In this paper our aim is to characterize the correlations of multiplex networks at the mesoscopic scale, and to use this information in order to build a network between the layers of multiplex datasets. In particular we propose an information theory measure $\tilde{\Theta}^S$, able to define similarities between the layers of a multiplex respect to their mesoscopic structures. This similarity is more significant when groups of nodes densely connected with each others are simultaneously present on different layers, forming overlapping communities. This measure is based on the concept of network entropy [23–25] and extends the Θ measure presented in [26]. Using the similarity $\tilde{\Theta}^S$, here we propose a method for extracting the network between the layers of multiplex networks. We apply the proposed method to the characterization of the American Physical Society (APS) Collaboration Multiplex Networks extracted from the APS dataset [27]. The scientific collaboration networks have been studied extensively in the context of single networks [28–32]. Nevertheless, additional relevant information can be extracted if they are analyzed as a multilayer structure [5, 6, 13]. The Collaboration Multiplex Networks are formed by the authors of the APS papers, and by layers corresponding to the Physics and Astronomy Classification Scheme (PACS) codes [33]. In particular two authors are linked on layer α if they have co-authored a paper with PACS code corresponding to layer α . Since the PACS codes are organized in

hierarchical levels we constructed two APS Collaboration Multiplex Networks corresponding to layers describing either the first or the second level of the PACS hierarchy. The analysis performed on the APS Collaboration Multiplex Networks has allowed us to characterize the network between the layers of these multiplex networks, and to investigate the same dataset at different levels of resolution with respect to the number of layers.

The paper is structured as follows: in Section II we define the indicator measure $\tilde{\Theta}^S$; in Section III we test the measure on two different multiplex benchmark models of two-layer network with communities; in Section IV we use our measure to analyze the community structure of the APS Collaboration Multiplex Network at two hierarchical levels of the PACS code; in Section V we compare the results obtained with $\tilde{\Theta}^S$ with results obtained using other similarity measures on the same dataset; finally in Section VI we give the conclusions.

II. DEFINITION OF $\tilde{\Theta}^S$

Our goal here is to construct an information theory indicator function $\tilde{\Theta}^S$ to characterize the similarity in the mesoscopic structure of the layers of a multiplex network. This indicator function is based on the entropy of network ensembles [23–26], a quantity which plays a key role when inference problems are addressed using an unbiased information theory approach [25, 26]. In this section we define how the indicator function $\tilde{\Theta}^S$ is defined. We consider a multiplex network formed by N nodes $i = 1, 2, \dots, N$ and M layers $\alpha = 1, 2, \dots, M$. The structure of the multiplex network is characterized by M adjacency matrices \mathbf{a}^α of elements $a_{ij}^\alpha = 1$ if node i is connected to node j in layer α , or $a_{ij}^\alpha = 0$ otherwise. We indicate with k_i^α the degree of a node i on layer α , i.e. the number of neighbors that node i has on α . The nodes having degree $k_i^\alpha = 0$ in layer α , are the isolated nodes, i.e. nodes that are not connected to any other node in the layer α , also called [6] in the context of multilayer networks “inactive” nodes in layer α . Conversely all the nodes with $k_i^\alpha > 0$ are called “active” nodes in layer α .

We assume that each node i of layer α has a characteristic $q_i^\alpha \in \{1, \dots, Q^\alpha\}$. The quantity q_i^α can for example indicate the community to which the node i belongs. More in general q_i^α can represent any feature of the nodes in layer α . Starting from this information we can classify the nodes in P^α classes $p_i^\alpha \in \{1, \dots, P^\alpha\}$ which take into account at the same time the information about the degree of the nodes and their characteristic q_i^α . This is the minimal assumption to capture the structure of networks with communities induced by the characteristics $q^\alpha = \{q_i^\alpha\}_{i=1,2,\dots,N}$, and strong heterogeneities in the degree. Considering only the partition induced by the characteristics would imply that in the network we do not consider the structure induced by the degrees, which is clearly not a viable option for broadly distributed networks.

Including other features of the nodes to define node classes could be a viable option. In this case the characteristics q^α will take into account different features which might depend on the specific network under consideration. Therefore here we take the class p_i^α to be a function of degree k_i^α and of the characteristic q_i^α , i.e. $p_i^\alpha = f(k_i^\alpha, q_i^\alpha)$. The block structure of the network induced by the classes $p_i^\alpha = f(k_i^\alpha, q_i^\alpha)$ is described by the matrices \mathbf{e}^α of elements $e^\alpha(p, p')$ indicating the total number of links on the layer α between nodes of class p and nodes of class p' . We define the entropy $\Sigma_{k^\alpha, q^\alpha}$ [23–26] of a layer α as the logarithm of the number of graphs preserving the block structure \mathbf{e}^α in a given layer. By considering the number of graphs preserving a given block structure, we have that this entropy takes the simple expression,

$$\Sigma_{k^\alpha, q^\alpha} = \log \left[\prod_{p < p'} \binom{n_p^\alpha n_{p'}^\alpha}{e^\alpha(p, p')} \prod_p \binom{n_p^\alpha (n_p^\alpha - 1)/2}{e^\alpha(p, p)} \right], \quad (1)$$

where

$$e^\alpha(p, p') = \sum_{i,j} a_{ij}^\alpha \delta[p_i^\alpha(k_i^\alpha, q_i^\alpha), p] \delta[p_j^\alpha(k_j^\alpha, q_j^\alpha), p'], \quad (2)$$

for $p \neq p'$, and $e(p, p), n(p)$ given respectively by

$$e^\alpha(p, p) = \sum_{i < j} a_{ij}^\alpha \delta[p_i^\alpha(k_i^\alpha, q_i^\alpha), p] \delta[p_j^\alpha(k_j^\alpha, q_j^\alpha), p], \quad (3)$$

and

$$n_p^\alpha = \sum_i \delta[p_i^\alpha(k_i^\alpha, q_i^\alpha), p], \quad (4)$$

with $\delta[x, y]$ indicating the Kronecker delta. The entropy $\Sigma_{k^\alpha, q^\alpha}$ is a measure to assess how much information is encoded in the constraint imposed to the network i.e. the block structure \mathbf{e}^α . The smaller is the entropy the smaller is the number of networks that share the block structure \mathbf{e}^α . Therefore the smaller is the entropy of an ensemble the larger is the level of information encoded by the constraint. If for a given assignment of the characteristics $\{q_i^\alpha\}$ the entropy is much smaller than in a random hypothesis (when the characteristics are reshuffled randomly between the nodes), then the network structure reflects the characteristic assignment $\{q_i^\alpha\}$ and thus the characteristics $\{q_i^\alpha\}$ capture relevant information respect to the network structure. Following this argument the quantity Θ proposed in [26], which is based on the entropy of network ensembles, has been shown to be an unbiased indicator able to quantify the specificity of a generic layer α to the assignment q_i^α . This information theory quantity is defined as:

$$\Theta_{k^\alpha, q^\alpha} = \frac{E_\pi[\Sigma_{k^\alpha, \pi(q^\alpha)}] - \Sigma_{k^\alpha, q^\alpha}}{\sqrt{E_\pi[(\Sigma_{k^\alpha, \pi(q^\alpha)} - E_\pi[\Sigma_{k^\alpha, \pi(q^\alpha)}])^2]}}, \quad (5)$$

where $E_\pi[\dots]$ is the expected value over random uniform permutations $\pi(q^\alpha)$ of the node characteristics q^α in layer α .

Here we propose to use this quantity to compare the similarity between the different layers in a multiplex network. Indeed we can consider the characteristics q^β of the nodes in layer β as an induced feature of nodes in layer α and measure by the corresponding indicator $\Theta_{k^\alpha, q^\beta}$ how much information the characteristics q^β contain respect to the node structure of layer α . In particular the indicator $\Theta_{k^\alpha, q^\beta}$ is given by

$$\Theta_{k^\alpha, q^\beta} = \frac{E_\pi[\Sigma_{k^\alpha, \pi(q^\beta)}] - \Sigma_{k^\alpha, q^\beta}}{\sqrt{E_\pi[(\Sigma_{k^\alpha, \pi(q^\beta)} - E_\pi[\Sigma_{k^\alpha, \pi(q^\beta)}])^2]}}. \quad (6)$$

Therefore $\Theta_{k^\alpha, q^\beta}$ measures the specificity of the layer α respect to the particular set q^β , which is the assignment of the characteristics of the nodes on layer β .

When one considers a single layer, the entropy is independent on the choice adopted for classifying isolated (inactive) nodes in layers belonging to multiplex networks. In fact, we can either group all the isolated nodes in a single class or each isolated node in a different class, and the entropy value given by Eq. (1) does not change because the isolated nodes have no links attached to them. Instead the indicator function $\Theta_{k^\alpha, q^\alpha}$ might depend on this choice because its construction involves several reshuffling of the characteristics of the nodes.

When comparing different layers of a multiplex network, the nodes that are active in one layer might not be active in another layer. Nevertheless, the information carried by the activity of the node might be significant. For example if two layers have very different activity patterns, it might occur that the nodes inactive in one layer form a well defined cluster in the other layer resulting in a very significant information that is important to capture. Therefore to distinguish between nodes active and inactive in a layer it is a very convenient choice to classify all the inactive nodes in one layer under a given common characteristic. A similar type of argument can be made about connected clusters of small sizes, which are “quasi-isolated” as the nodes belonging to connected clusters of size 2 or 3 etc. Depending on the number of such clusters it might be convenient to classify also nodes in connected components of size 2 or 3 etc. into given common characteristics as we will show in the next sections using the concrete examples of the APS Collaboration Multiplex Networks. Here, if not stated otherwise, we will consider the case in which the features q^α indicates the community of the nodes in layer α and the characteristic p_i^α takes a different value for each distinct pair (k_i^α, q_i^α) where $k_i^\alpha \neq 0$, while all the nodes with $k_i^\alpha = 0$ form another class of nodes.

In order to compare the level of information carried in layer α by the community structure in layer β , q^β , with the level of information carried by the proper community

structure, q^α , we define the quantity

$$\tilde{\Theta}_{\alpha, \beta} = \frac{\Theta_{k^\alpha, q^\beta}}{\Theta_{k^\alpha, q^\alpha}}. \quad (7)$$

The quantity $\tilde{\Theta}_{\alpha, \beta}$ is a measure of how layer β is similar to α respect to the community assignment \mathbf{q} . If $\tilde{\Theta}_{\alpha, \beta} = 1$ the community structure q^β , proper of layer β , carries the same level of information for the structure of layer α as the community structure q^α , proper of the layer α . It is important to notice that the matrix $\tilde{\Theta}$ in principle is not symmetric. We can construct the symmetric measure $\tilde{\Theta}_{\alpha, \beta}^S$ by symmetrizing the quantity $\tilde{\Theta}_{\alpha, \beta}$ i.e. by defining

$$\tilde{\Theta}_{\alpha, \beta}^S = \frac{\tilde{\Theta}_{\alpha, \beta} + \tilde{\Theta}_{\beta, \alpha}}{2}. \quad (8)$$

This is a symmetric measure indicating how similar layer α and layer β are with respect to their community structure. In Figure 1 we give a schematic summary of the method used to construct the similarity measure $\tilde{\Theta}_{\alpha, \beta}^S$.

In a given multiplex network, we can then analyze the entire symmetric matrix $\tilde{\Theta}^S$ measuring the similarity between the community structure of the layers. This matrix characterizes the entire multiplex network at the layer level, reducing the information about the network structures to one matrix of similarity between the layers.

In the following Section we will first test this measure on multiplex network benchmark models with non trivial community structure, then in the subsequent Section we will focus on characterizing the APS Collaboration Multiplex Networks where the layers are the collaborations networks of scientists using different PACS numbers.

In this paper we are mostly concerned about similarities in the community structure of the layers of a multiplex network, nevertheless it has to be stressed that the proposed approach and similarity measure $\tilde{\Theta}_{\alpha, \beta}^S$ is general and it can be used by considering any available feature of the nodes related to the structure of the layers.

III. TESTING $\tilde{\Theta}^S$ ON BENCHMARK MODELS

In order to validate on a well defined multiplex architecture our similarity measure $\tilde{\Theta}^S$ respect to the community structures of different layers of a multiplex network, we have developed two benchmark models with communities. In particular we want to construct benchmark multiplex network models with a controlled level of overlap between the communities in different layers. Given in a generic multilayer the community assignment q^α of the nodes on each layer α , we define the community overlap as

$$O_c = \frac{2}{M(M-1)} \frac{1}{N} \max_{\{\pi\}} \left\{ \sum_{\alpha < \beta} \sum_{i=1}^N \delta[q_i^\alpha, \pi(q_i^\beta)] \right\}, \quad (9)$$

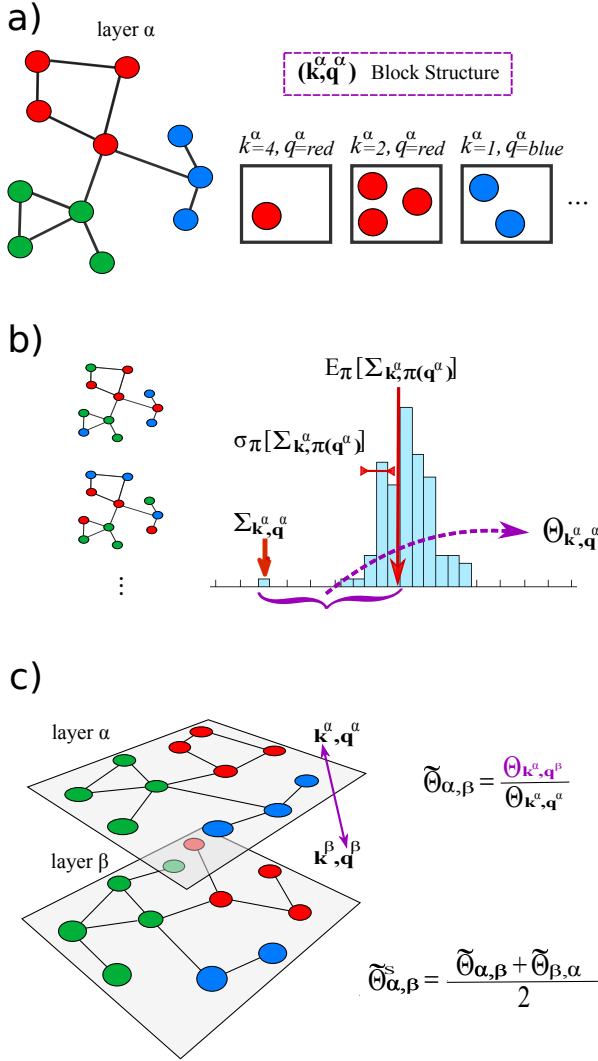


FIG. 1: (Color online) Diagram showing the method. Panel a): We consider a layer α in a multiplex network and we define the node classes $p^{\alpha} = (k^{\alpha}, q^{\alpha})$, where k^{α} indicates the node degrees and q^{α} the node characteristics on the layer α . These classes induce a block structure in the network specified by the number of links between the nodes of each class and the number of links connecting the nodes in different classes. Panel b): The entropy $\Sigma_{\mathbf{k}, \mathbf{q}}^{\alpha}$ given by Eq. (1) is calculated and compared with the entropy distribution obtained in a random hypothesis, by performing random uniform permutations $\pi(q^{\alpha})$ of the characteristics q^{α} of the nodes and subsequently measuring the $\Sigma_{\mathbf{k}, \mathbf{q}}^{\alpha}$ values. The mean $E_{\pi}[\Sigma_{\mathbf{k}, \mathbf{q}}^{\alpha}]$ and standard deviation $\sigma_{\pi}[\Sigma_{\mathbf{k}, \mathbf{q}}^{\alpha}]$ of the entropy distribution is thus calculated. The indicator function $\Theta_{\mathbf{k}, \mathbf{q}}^{\alpha}$ measures the difference between $\Sigma_{\mathbf{k}, \mathbf{q}}^{\alpha}$ and $E_{\pi}[\Sigma_{\mathbf{k}, \mathbf{q}}^{\alpha}]$ in units of $\sigma_{\pi}[\Sigma_{\mathbf{k}, \mathbf{q}}^{\alpha}]$. Panel c): Given a second layer β , $\tilde{\Theta}_{\alpha, \beta}$ characterizes the information about the structure in layer α , carried by the characteristics of nodes in layer β . In order to define a symmetric indicator function of the similarity between the layers α and β we define the indicator $\tilde{\Theta}_{\alpha, \beta}^S$ that symmetrizes the indicator function $\tilde{\Theta}_{\alpha, \beta}$.

where M indicates the total number of layers and N indicates the total number of nodes, $\delta[x, y]$ indicates the Kronecker delta and the maximum is taken over all the permutations $\pi(q^{\beta})$ of the label of the communities in layer β .

We define two benchmark models (see Figure 2) based respectively on the Girvan and Newman (GN) [34] model and on the Lancichinetti - Fortunato - Radicchi (LFR) model [35], which are very well established benchmarks for single networks with communities. The proposed benchmarks are designed to tune the overlap of communities between different layers of simple multiplex networks having respectively homogeneous or heterogeneous degree distribution and community size distribution.

For the first benchmark model, the Duplex Network GN model (DNGN) we construct a duplex network (a multiplex network made of two layers) in which each layer is formed by a GN network realization. Therefore each of the layers is formed by N nodes divided into 4 equal size clusters of size N_c .

The network in each layer is a random network in which each node has a probability p_{in} to link to nodes of its same community and a probability p_{out} to link to nodes outside its community. In particular we have chosen p_{in} and p_{out} in order to have for each node, a mean degree $\langle k \rangle = 16$ and a mean number of links outside the community given by $\langle k_{out} \rangle = 4$. The layers generated in this way have a well defined community structure and they are essentially random respect to other network characteristics. The characteristic q_i^{α} indicates the community to which a node i belongs on layer $\alpha = 1, 2$. Here we consider the possible correlations existing between the community assignment $q_i^{[1]}$ and $q_i^{[2]}$ in the two layers. This community assignment allows us to tune in a control way the level of overlap between the communities. In particular we label the nodes $i = 1 \dots, N$ in layer 1 according to the following community assignment q_i^{α} ,

$$q_i^{[1]} = \left\lceil \frac{i}{N_c} \right\rceil. \quad (10)$$

where the brackets $\lceil x \rceil$ in the right end side of this expression indicate the ceiling function of x . Therefore we have, for $N = 128$ and $N_c = 32$,

$$q_i^1 = \begin{cases} 1 & \text{for } i \in [1, 32] \\ 2 & \text{for } i \in [33, 64] \\ 3 & \text{for } i \in [65, 96] \\ 4 & \text{for } i \in [97, 128] \end{cases}.$$

The community assignment in layer 2 will not be in general the same of layer 1. In order to model overlap of communities we perform a simple “shift” of the labels, parametrized with the parameter $\rho > 0$. In particular we take

$$q_i^{[2]} = \begin{cases} \left\lceil \frac{i - \rho N_c}{N_c} \right\rceil & \text{if } \left\lceil \frac{i - \rho N_c}{N_c} \right\rceil > 0 \\ \frac{N}{N_c} & \text{if } \left\lceil \frac{i - \rho N_c}{N_c} \right\rceil = 0 \end{cases}.$$

In general the control parameter ρ takes values $0 \leq \rho \leq 0.5$. If $\rho = 0$ there is no “shift” between the layer partitions (they perfectly match); if $\rho > 0$ each community in the first layer overlaps with the corresponding one in the second layer for a fraction of nodes equal to $(1 - \rho) \cdot N_c$; thus $\rho \cdot N_c$ is the number of “shifted” nodes per community. When $\rho = 0.5$, $N = 128$ and $N_c = 32$, we have

$$q_i^2 = \begin{cases} 1 & \text{for } i \in [17, 48] \\ 2 & \text{for } i \in [49, 80] \\ 3 & \text{for } i \in [81, 112] \\ 4 & \text{for } i \in [1, 16] \cup [113, 128] \end{cases}.$$

Therefore $\rho = 0.5$ describes the maximum “shift” between the community of the two layers: each community in the first layer shares 16 nodes with its corresponding community in the second layer. Given a value of ρ the overall community overlap in the network can be easily calculated, being $O_c = (1 - \rho)$, and in the case of maximum “shift” we obtain $O_c = 0.5$.

For the second benchmark model the Duplex Network LFR model (DNLFR), we have taken a duplex network in which the single layers are constructed according to the LFR model [35].

1. The network in the first layer is a LFR network, formed by Q communities. The communities are labelled according to their size in descending order.
2. The network in the second layer is a LFR network with Q communities generated using the same parameters used for the network in the first layer. Additionally we require that the network in the second layer satisfies a further condition, which allows us to modulate the overlap between the communities in the two layers. Specifically, for each second layer candidate, we first label the communities according to their size in descending order. Then we compare each of them to the corresponding one in the first layer (panel B Figure 2). We calculate the number of “shifted” nodes N_s given by the sum of the absolute values of the difference between the corresponding communities sizes, i.e.

$$N_s = \sum_{l=1}^Q \left| n_l^{[1]} - n_l^{[2]} \right|, \quad (11)$$

where n_l^α is the size of the community l in layer α . Finally we retain the candidate network as the second layer of the duplex network only if

$$\lfloor (\rho - \Delta\rho) \cdot S_{min} \rfloor \leq N_s < \lfloor (\rho + \Delta\rho) \cdot S_{min} \rfloor, \quad (12)$$

where $\lfloor \dots \rfloor$ is the floor function. Here ρ and $\Delta\rho$ are control parameters of the benchmark model that modulate the overlap of the communities, and S_{min} in Eq. (12) is the parameter that in the LFR model fixes the lower bound of the community sizes.

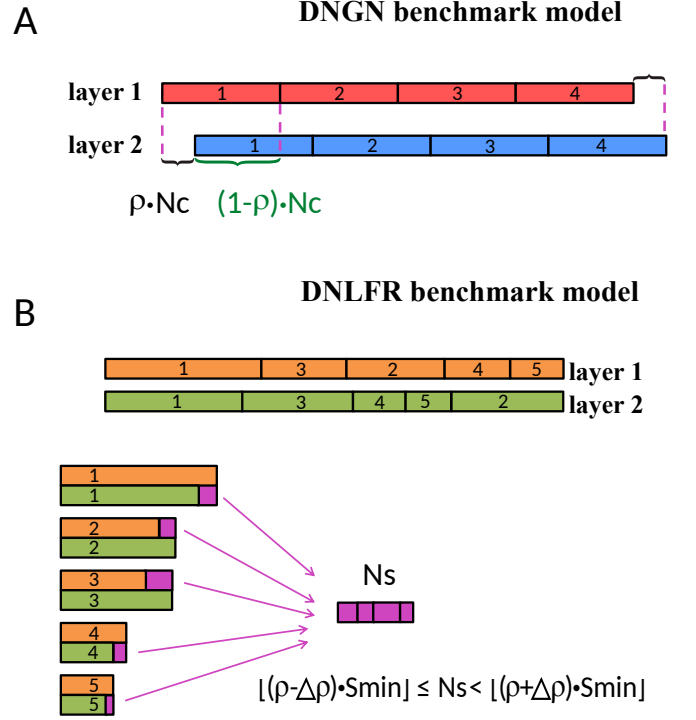


FIG. 2: (Color online) Schematic of the benchmark models DNGN and DNLFR. Panel (A). The DNGN benchmark model: nodes on both layers (blue and red) are divided into four communities of equal size N_c , labelled from 1 to 4. Each community of layer 1 overlaps for a fraction of $(1 - \rho) \cdot N_c$ nodes with its corresponding community in layer 2. Panel (B). The DNLFR benchmark model: on each layer $Q = 5$ non homogeneous communities are generated and labelled from 1 to 5 according to their size (left). For a given ρ the total number of nodes which do not overlap between communities of the same label, N_s , has values $\lfloor (\rho - \Delta\rho) \cdot S_{min} \rfloor \leq N_s < \lfloor (\rho + \Delta\rho) \cdot S_{min} \rfloor$, where $\lfloor \dots \rfloor$ is the floor function and S_{min} is the minimum bound of the power-law distribution from which the community sizes in the two layers are extracted.

In this way if one considers a sufficient number of multiple realizations of the multilayer, and a sufficiently low value of $\Delta\rho$, one gets

$$\langle N_s \rangle \simeq \lfloor \rho \cdot S_{min} \rfloor. \quad (13)$$

3. Finally, the nodes are relabelled in both layers in order to allow the maximum community overlap. In particular the labels are reassigned in such a way that the common number of nodes in the communities that have the same label in the two layers, is equal to the minimum of the two community sizes. (see Figure 2.)

Therefore the average community overlap of the benchmark network is dependent on ρ and, for a significant number of realizations and low enough values of $\Delta\rho$, is given by

$$\langle O_c \rangle = 1 - \frac{\langle N_s \rangle}{N} \simeq 1 - \frac{\lfloor \rho \cdot S_{min} \rfloor}{N}. \quad (14)$$

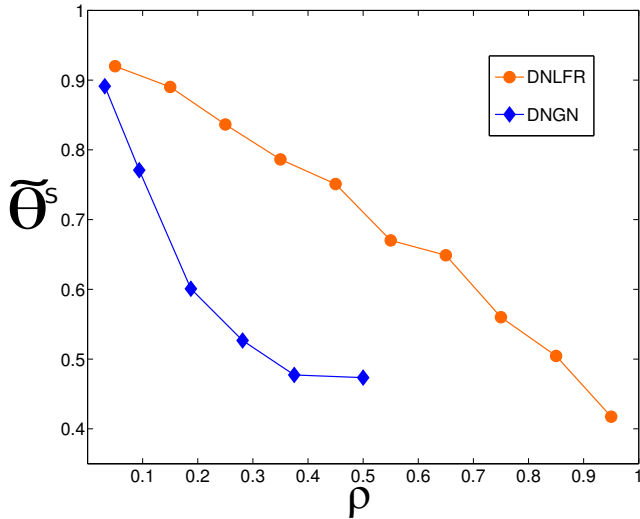


FIG. 3: (Color online) The similarity measure $\tilde{\Theta}^S$ between the two layers of the DNGN (blue diamonds) and DNLFR (orange circles) benchmark models is measured as a function of the control parameter ρ . When ρ increases the total community overlap between the layers decreases and $\tilde{\Theta}^S$ decreases monotonically both in the case of homogeneous-size communities (DNGN) and in the case of heterogeneous-size communities (DNLFR). Each data point is averaged over 50 benchmark realizations. For the DNLFR model the parameter $\Delta\rho$ was set to 0.05.

In order to test the performance of the similarity measure $\tilde{\Theta}^S$, we apply this measure to the two duplex network benchmarks, for different values of ρ . Since ρ modulates the level of community overlap between the layers we expect that the similarity measure $\tilde{\Theta}^S$ is larger for lower value of ρ (corresponding to larger community overlap O_c between the layers) and smaller for larger values of ρ (corresponding to smaller community overlap O_c between the layers). In Figure 3 we show the dependence $\tilde{\Theta}^S$ as a function of ρ for the two proposed benchmark models. In both cases the displayed values $\tilde{\Theta}^S$ are averaged over 50 benchmark realizations.

For the DNGN benchmark, we considered $N = 128$, $N_c = 32$ and $\rho \leq 0.5$. The similarity measure $\tilde{\Theta}^S$ is monotonically decreasing with ρ . For the DNLFR benchmark the two single layers are generated according to the LFR algorithm with parameters $N = 600$ (number of nodes) and $Q = 5$ (number of communities). The size of each community is taken from a power-law distribution with lower bound $S_{min} = 60$, upper bound $S_{max} = 180$, and power-law exponent $\tau_1 = 1.5$. Inside the communities the node degree distribution is also extracted from a power-law distribution with parameters $k_{max} = 50$ (maximum degree), $\tau_2 = 2.6$ (power-law exponent), $\langle k \rangle = 16$ (average degree). For building the DNLFR network we used $\Delta\rho = 0.05$ and $\rho \leq 0.95$. Also in the case of the DNLFR benchmark, where the size of the communities is heterogeneous, $\tilde{\Theta}^S$ decreases monotonically with ρ .

This result shows that in benchmark models in which

the community overlap is modulated by an external control parameter, $\tilde{\Theta}^S$ decreases together with the community overlap. Since in general measuring the community overlap involves an optimization over a permutation of the community assignment, measuring the community overlap can be very costly numerically. In this situation calculating $\tilde{\Theta}^S$ could instead give an alternative way to assess the similarity between the layers of a multiplex network.

In Section V, using the concrete examples of the APS Collaboration Multiplex Networks, we will compare the similarity measure $\tilde{\Theta}^S$ to other existing measures introduced to compare different community assignments in single layers.

IV. THE NETWORK BETWEEN THE LAYERS OF THE APS COLLABORATION MULTIPLEX NETWORKS

In this Section, we use the similarity matrix $\tilde{\Theta}^S$ to analyze the APS Collaboration Multiplex Networks. These multiplex networks are extracted from the APS collaboration dataset [27] recording all the bibliometric information about the papers published in the APS journals.

The network is formed by a set of N nodes representing the APS authors. Since there is no agreement on disambiguation techniques for the author names, we have identified each author with the initials of his/her first name and last name. The layers correspond to different Physics and Astronomy Classification Scheme (PACS) codes [33] describing the subject of the papers. Two authors are linked in a given layer α if they are co-authors of at least one paper having the PACS number corresponding to layer α . Since PACS numbers are organized in a hierarchical way (the first digit of the number indicates the general field of physics while the second digit specifies the ambit inside that field), we have constructed two multiplex networks whose layers correspond respectively to the first and second hierarchical level of the PACS codes. The APS Collaboration Multiplex Network related to the first level of the hierarchy of PACS codes is made of $M_1 = 10$ layers each one describing the collaboration network in a general field of physics. The APS Collaboration Multiplex Network at the second level of the hierarchy is made of $M_2 = 66$ layers each one describing the collaboration network in a specific ambit of physics (second level of the PACS code hierarchy).

In extracting the APS Collaboration Multiplex Networks we considered all the papers until 2014 with less than ten co-authors. This threshold was introduced to exclude papers coming from big collaborations that follow different statistical properties with respect to the rest of the dataset. With this threshold, our dataset includes a consistent fraction of the whole dataset ($\simeq 97\%$ of the total number of papers) and a number of authors $N = 180,539$.

The layers of the APS Collaboration Multiplex Net-

works are characterized by a significantly different activity pattern of the nodes. Moreover roughly 0.7% of nodes belong to connected components of size 2 while only about 0.006% of the nodes belongs to connected components of size 3. Therefore we consider here the case in which the characteristics $\{q_i^\alpha\}$ indicate the community of the nodes in layer α and the class p_i^α of node i in layer α takes a different value for each distinct pair (k_i^α, q_i^α) as long as the node i is not isolated $k_i^\alpha > 0$, and it belongs to a community of more than two nodes. All the isolated nodes belong a the same class \tilde{p} . All the nodes belonging to a two-node community belong to another class \tilde{p} .

Let us first characterize the mesoscale similarities between the $M_1 = 10$ layers of the APS Collaboration Multiplex Network in the main subjects of physics, described by the first level of the PACS code hierarchy. The similarity matrix $\tilde{\Theta}^S$ is constructed in two different ways, using either the Infomap community detection algorithm [36] and the Louvain algorithm [37], and averaging in both cases over 350 random permutations of the community assignments. For simplicity we will refer to these two matrices as Infomap- $\tilde{\Theta}^S$ and Louvain- $\tilde{\Theta}^S$. The two matrices are reported in Figure 4 in the form of heat-maps. The patterns shown by the two heat-maps are very similar, denoting that from a qualitatively point of view the measure $\tilde{\Theta}^S$ is not affected by the choice of the algorithm used to perform the community detection for the network under study. We can observe that, in general, clusters in the APS Collaboration Multiplex Network extend across multiple layers. As expected, layers describing collaborations in general or interdisciplinary fields such as General Physics or Interdisciplinary Physics, which often involve people from different specific ambits of physics, show high values of $\tilde{\Theta}^S$ respect to several other layers while more specific fields, such as Gases&Plasma, show lower values of $\tilde{\Theta}^S$ respect to the other layers.

Given this similarity measure between the layers of the multiplex, one can build a network of networks whose nodes represent the $M_1 = 10$ networks of collaboration in general fields of physics and whose weighted edges are the values $\tilde{\Theta}_{\alpha,\beta}^S$ and represent the similarity between the M_1 networks respect to their community structure. This network of layers is thus a weighted fully-connected network showing itself a significant community structure and revealing how the pattern of collaboration between scientists is organized across different fields of physics. In order to characterize this community structure between the layers of the multiplex network, we perform a hierarchical clustering analysis starting from the dissimilarity matrix d of elements $d_{\alpha,\beta}$ given by

$$d_{\alpha,\beta} = 1 - \left| \tilde{\Theta}_{\alpha,\beta}^S \right|. \quad (15)$$

Specifically, we use the average linkage clustering method which gave the best cophenetic correlation coefficient compared to other clustering methods[38–40]. According to the average method the distance $d_c(C_1, C_2)$ between

two clusters C_1 and C_2 is defined as the average distance between all pairs of layers in the two clusters:

$$d_c(C_1, C_2) = \frac{1}{\mathcal{N}(C_1)\mathcal{N}(C_2)} \sum_{\alpha \in C_1} \sum_{\beta \in C_2} d_{\alpha,\beta} \quad (16)$$

where $\mathcal{N}(C_i)$ indicates the number of layers in cluster C_i .

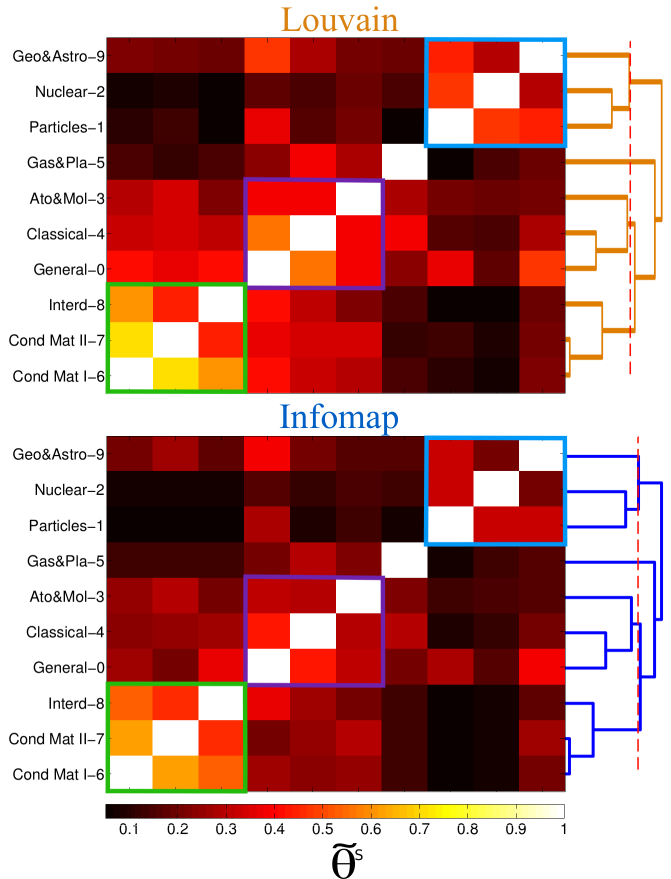


FIG. 4: (Color online) The similarity matrices of elements $\tilde{\Theta}_{\alpha,\beta}^S$ calculated respectively using the Louvain and the Infomap community detection algorithms are plotted for the APS Collaboration Multiplex Network with the $M_1 = 10$ layers indicating the collaboration network at the first level of the PACS hierarchy. Each layer refers to a general field of Physics (see Table I for the legend of the layer acronyms). The dendrogram between the layers is shown on the left of each matrix $\tilde{\Theta}_{\alpha,\beta}^S$. The dashed line on top of the dendrogram indicates the partition that correspond to the optimal value of the weighted modularity given by Eq. (17).

In Figure 4, together with the matrices Infomap- $\tilde{\Theta}^S$ and Louvain- $\tilde{\Theta}^S$ we show the dendrograms resulting from the hierarchical clustering analysis of the respective dissimilarity matrices Infomap- d and Louvain- d . In order to define an optimal partition of the layers into communities, we looked for the agglomerative stage of the cluster hierarchy at which the weighted modularity Q [41] is

Acronym	PACS	Field
General-0	00	General
Particles-1	10	Physics of Elementary Particles and Fields
Nuclear-2	20	Nuclear Physics
Ato&Mol-3	30	Atomic and Molecular Physics
Classical-4	40	Electromagnetism, Optics, Acoustic, Heat Transfer, Classical Mechanics and Fluid Dynamics
Gas&Pla-5	50	Physics of Gases, Plasmas and Electric Discharges
Cond Mat I-6	60	Condensed Matter: Structural, Mechanical and Thermal Properties
Cond Mat II-7	70	Condensed Matter: Electronic Structure, Electrical, Magnetic and Optical properties
Interd-8	80	Interdisciplinary Physics and Related Areas of Science and Technology
Geo&Astro-9	90	Geophysics, Astronomy and Astrophysics

TABLE I: The acronyms used in this study for the PACS number at the first level of the PACS hierarchy, the corresponding PACS numbers and corresponding general fields of Physics.

maximized, Q defined as:

$$Q = \frac{1}{\langle \eta \rangle M} \sum_{\alpha \neq \beta}^M \left(\left| \tilde{\Theta}_{\alpha, \beta}^S \right| - \frac{\eta_{\alpha} \eta_{\beta}}{\langle \eta \rangle M} \right) \delta[\sigma_{\alpha} \sigma_{\beta}], \quad (17)$$

where σ_{α} labels the community in which layer α is, $\delta[x, y]$ indicates the Kronecker delta and η_{α} , $\langle \eta \rangle$ are given respectively by

$$\begin{aligned} \eta_{\alpha} &= \sum_{\beta \neq \alpha} \left| \tilde{\Theta}_{\alpha, \beta}^S \right|, \\ \langle \eta \rangle &= \frac{1}{M} \sum_{\alpha} \eta_{\alpha}. \end{aligned} \quad (18)$$

As shown in Figure 4 the optimal partition found is the same either when using the Infomap algorithm or the Louvain algorithm to perform the community detection in the layers of the multiplex. The analysis reveals that the first layers clustering together are Condensed Matter I&II and Interdisciplinary Physics and they form the first block (green coloured box); the second block includes General Physics, Classical Physics, Atomic and Molecular Physics (purple coloured box); in the third block Particles Physics, Nuclear Physics and Geophysics&Astrophysics group together (cyan coloured box). The layer related to Gases&Plasma Physics is isolated and can be considered as a block by itself.

Once revealed the block (community) structure an interesting issue is to characterize the Minimal Spanning

Tree (MST) that allows us to identify the layers which connect the blocks together. Therefore we construct the MST using the dissimilarity measure d defined in Eq. (15) calculated either using the Infomap or the Louvain clustering algorithm. The two MSTs are identical (Figure 5) and this confirm the robustness of the results with respect to the community detection algorithm used. We can see that the collaboration layer of General Physics connects the three main blocks together.

Block 1	Block 2	Block 3	Block 4
Cond Mat I-6 Cond Mat II-7 Interd-8	General-0 Ato&Mol-3 Classical-4	Particles-1 Nuclear-2 Geo&Astro-9	Gas&Pla-5

TABLE II: Clusters between the $M_1 = 10$ layers of the APS multiplex network corresponding to the first level of the PACS hierarchy (see for the legend of the layer acronym Table I). The clusters have been obtained from the dendrograms shown in Figure 4, cut in order to obtain the partition that optimizes the weighted modularity Q defined in Eq. (17).

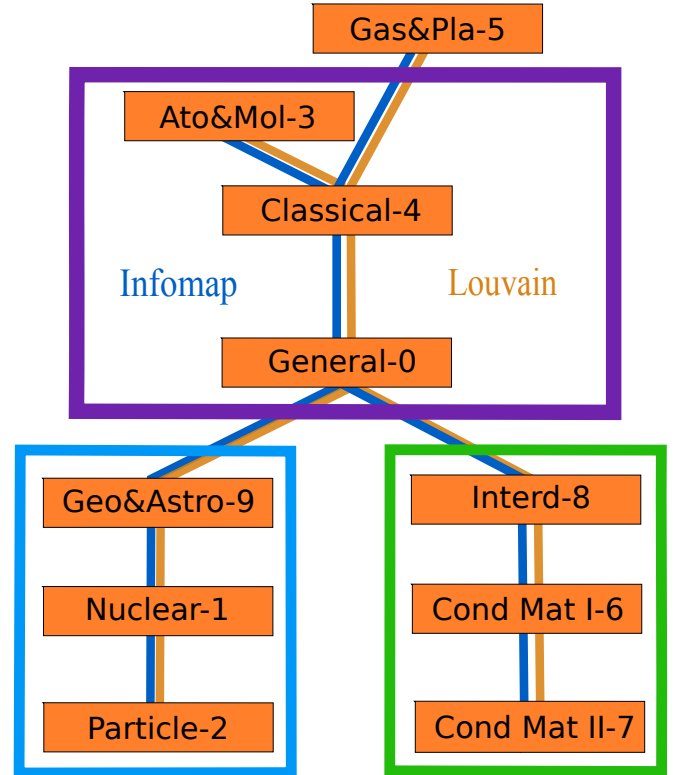


FIG. 5: (Color online) Minimal Spanning Tree (MST) using the dissimilarity measure d in the case of Infomap- d dissimilarity (blue) and in the case of Louvain- d dissimilarity (ocher). The block structure obtained with the hierarchical clustering analysis is also showed.

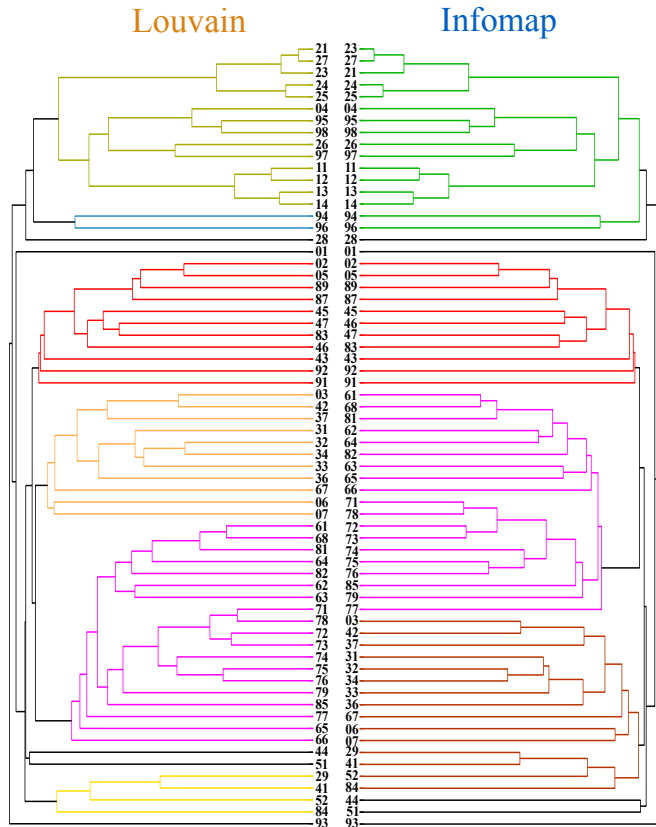


FIG. 6: (Color online) Hierarchical clustering of the APS Collaboration Multiplex Network in which each layer represents a collaboration network in a specific area of physics, as described by the second hierarchical level of the PACS code. We show the two dendrograms obtained respectively from the Louvain- $\tilde{\Theta}_{\alpha,\beta}^S$ (left) and from the Infomap- $\tilde{\Theta}_{\alpha,\beta}^S$ (right). In each dendrogram the communities found at the optimal partition (maximum of Q) are represented as branches of the same colors.

In order to have a deeper understanding of the results previously found we now consider the multiplex network of scientific collaborations where the layers are related to the PACS code at the second level of the PACS hierarchy. For this multiplex network we have calculated the similarity matrix $\tilde{\Theta}^S$ between the $M_2 = 66$ layers and found the optimal partition into communities according to the score function Q , following an analogous procedure to the one used previously for first level of the PACS hierarchy. To calculate $\tilde{\Theta}_{\alpha,\beta}^S$ we have performed averages over 350 random permutations of the community assignments.

In Figure 6 we plot the dendrograms resulting from the hierarchical clustering analysis in the case of Louvain- d dissimilarity and Infomap- d dissimilarity. For each dendrogram, the clusters found in the optimal partitions are represented as branches of the same colors. When using the Louvain- d dissimilarity we obtain six clusters plus some isolated layers. When using the Infomap- d dissimilarity we obtain four clusters plus isolated layers. Nevertheless we observe that two of the clusters (the red and the violet clusters) are identically the same in the two partitions. The other two clusters obtained with the Infomap- d dissimilarity are each divided into two clusters when considering the optimal partition using the

Louvain- d dissimilarity. In particular the combination of the green-yellow and green-blue clusters in the Louvain partition is identical to the green cluster of the Infomap partition, while the combination of the orange and the yellow clusters in the Louvain algorithm is identical to the brown cluster of the Infomap partition.

In Figure 7 we give an overview of the blocks hierarchy found. The four clusters found in the Infomap- d optimal partition matrix are represented by solid-line ovals. Dashed ovals split two clusters in two, according to the results obtained from the Louvain- d optimal partition. The block structure at the first level of the PACS hierarchy is shown using solid-line polygons. This method allows us to characterize with a bottom-up method how the organization of knowledge in physics is effectively perceived by scientists while shaping their collaboration network. We observe that while the PACS hierarchy clearly captures main features of the collaboration network, the analysis of the Collaboration Multiplex Network at the second level of the PACS hierarchy clearly suggests a hierarchical organization of these PACS numbers that is not equivalent to the first level of the PACS hierarchy. Finally we used the information gained by this analysis to construct the network of networks between the lay-



FIG. 7: (Color online) Optimal community structure of the layers of the APS Collaboration Network in which each layer represents a collaboration network in a specific area of physics, as described by the second hierarchical level of the PACS code. The four communities found starting from the Infomap- $\tilde{\Theta}_{\alpha,\beta}^S$ matrix are represented by blue solid-line ovals. In the partition obtained from the Louvain- $\tilde{\Theta}_{\alpha,\beta}^S$ two sub-communities (other dashed ovals) are considered separate communities. These communities form the coarse-grained partition into the three blocks found at the first hierarchical level of the PACS code (colored solid-line polygons). The nodes displayed in this figure correspond to a subset of 61 layers that are not isolated in the optimal partition in communities which optimizes the weighted modularity Q .

ers of the Collaboration Multiplex Network at the second level of the PACS hierarchy. To this aim we have constructed the weighted network determined by an opportune thresholding of the Louvain- $\tilde{\Theta}_{\alpha,\beta}^S$ or Infomap- $\tilde{\Theta}_{\alpha,\beta}^S$ similarity matrix (see Figure 8). The threshold, is here given by the minimum value of the similarity matrix $\tilde{\Theta}^S$ that ensures that each layer is connected to at least one other layer of its own cluster. From these networks, it is possible to appreciate that, although the network between the layer of the Collaboration Mutliplex Network is

highly interconnected, the clusters found corresponds to layers much more similar between themselves than with other layers outside their own cluster. Interestingly this visualization shows that the two clusters detected only by the Louvain algorithm, [94, 96] and [29, 41, 52, 84], contain the nodes that act as bridges between the yellow-green cluster and the red and the orange clusters. This might explain why the Louvain algorithm identifies them as separate clusters.

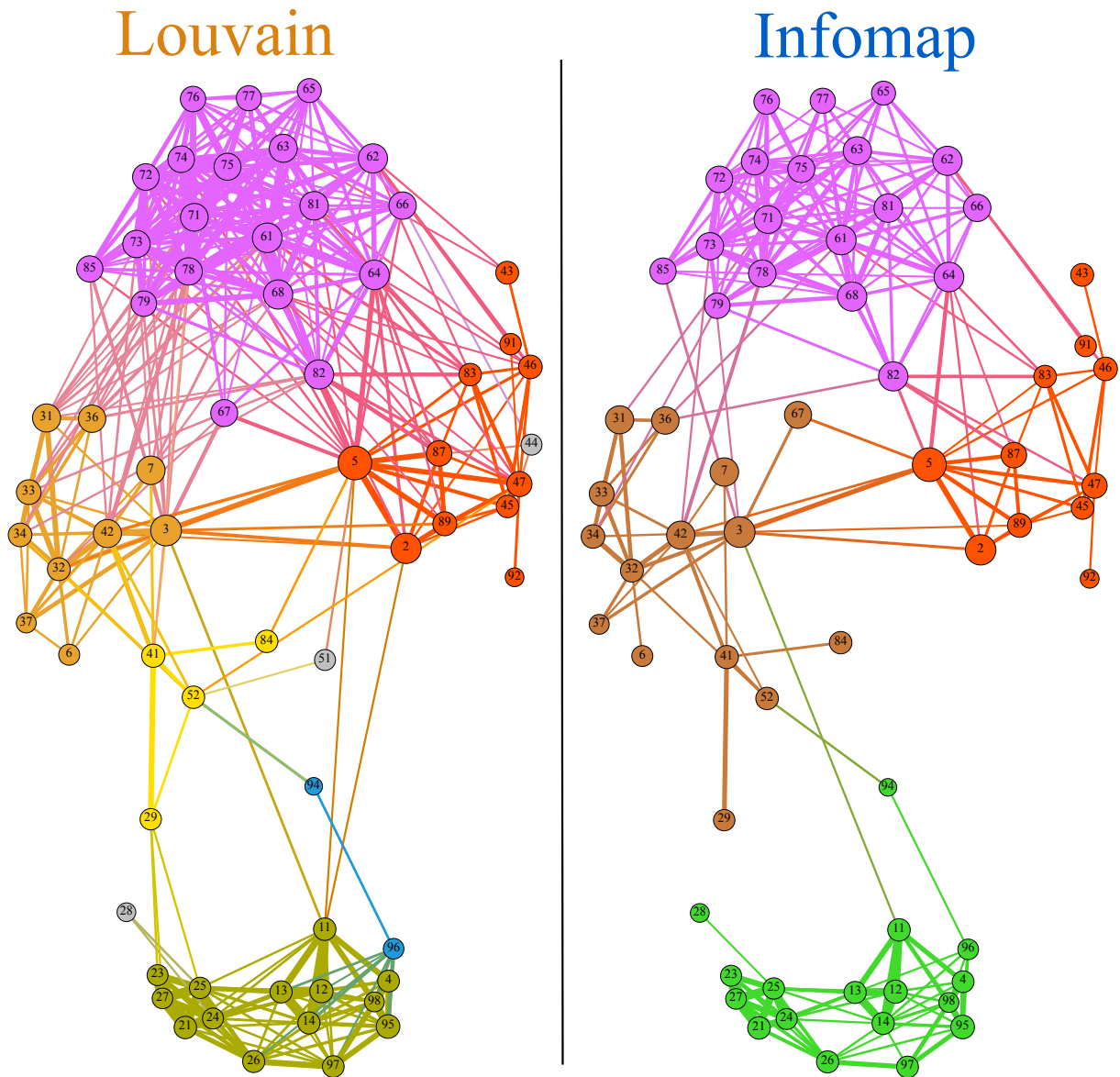


FIG. 8: (Color online) The network between the layers of the APS Collaboration Multiplex Network (with layers corresponding to the PACS code at the second level of the PACS hierarchy) is displayed here for the two cases in which the Louvain- $\tilde{\Theta}^S$ or the Infomap- $\tilde{\Theta}^S$ similarity matrix are used. The link weights represent the similarity between the community structure of the two linked layers. The networks are obtained from the $\tilde{\Theta}^S$ similarity matrix by filtering out the links below a given threshold value. The threshold is chosen to be the maximal value that ensures that in the filtered network each layer is connected with at least one layer inside its own cluster. The architecture of the networks describes the interplay between the collaboration networks and the organization of knowledge in physics. The community structure revealed by the hierarchical clustering analysis is shown making use of the same color scheme of Figure 6.

V. COMPARISON OF THE RESULTS OBTAINED WITH $\tilde{\Theta}^S$ RESPECT TO OTHER SIMILARITY MEASURES

In this Section we compare the results obtained from the analysis of the APS Collaboration Multiplex Network using the $\tilde{\Theta}^S$ indicator with results from other similarity measures commonly used to compare different network partitions [17] and with the *ACTIVIS* Index, an index

able to capture the similarity of the layers of a multiplex due to the activity of the nodes. In particular, focusing on the highest level of the PACS hierarchy, we compute the Normalized Mutual Information NMI [45], the Jaccard index J [42], the Rand index R [43, 44] and the *ACTIVIS* Index for each pair of the $M_1 = 10$ layers. Given two network partitions X and Y , the Normalized

Mutual Information NMI , is defined as

$$NMI(X, Y) = \frac{2[H(X) - H(X|Y)]}{H(X) + H(Y)}, \quad (19)$$

where $H(X) = -\sum_x P(x) \log P(x)$ is the entropy associated to the distribution $P(x)$ of sizes x of the clusters classified by the partition X ; $H(Y)$ corresponds to the entropy associated to the distribution $P(y)$ of the sizes y of the clusters in the partition Y ; $H(X|Y)$ is the conditional entropy associated to the distribution of the community assignment X conditioned on the distribution of the community assignment Y and is given by $H(X|Y) = -\sum_{x,y} P(x, y) \log P(x, y)/P(y)$, $P(x, y)$ the distribution of the number of nodes having community assignment x in partition X and y in partition Y .

The Jaccard index J and the Rand Index R , are instead defined as

$$J(X, Y) = \frac{a_{11}}{a_{11} + a_{10} + a_{01}},$$

$$R(X, Y) = \frac{a_{11} + a_{00}}{a_{11} + a_{10} + a_{01} + a_{00}}, \quad (20)$$

where a_{11} is the number of pairs of nodes belonging to the same cluster in both partitions X and Y , a_{00} is the number of pairs of nodes classified in different clusters in both the X and Y partitions, and $a_{10}(a_{01})$ is the number of pair of nodes belonging to the same cluster in $X(Y)$ but belonging to different clusters in $Y(X)$.

Finally we define the Activity Similarity *ACTIVIS* Index between the layers α and β of a multiplex network, which compares the activity patterns in different layers. This index is given by

$$ACTIVIS = b_{11} + b_{00}, \quad (21)$$

where b_{11} are the fraction of nodes active in both layers and b_{00} are the fraction of nodes inactive in both layers.

In Figure 9 we show the similarity matrices for the different measures and their respective dendrograms, obtained with the same hierarchical clustering analysis discussed above for the $\tilde{\Theta}^S$ case. Here the layer partitions are obtained using the Infomap algorithm. When the modularity Q is optimized, the partition obtained with all these alternative measures are different from the one obtained using the $\tilde{\Theta}^S$ indicator function. Moreover the partitions obtained are characterized by having at least

3 out of 10 layers in separate clusters, resulting in significantly less relevant partitions. Moreover, by looking at the dendrograms, we can see that none of the other measure is able to give the optimal partition obtained with $\tilde{\Theta}^S$ even by applying an arbitrary cut to the respective dendrogram.

These results show clearly that the proposed indicator function $\tilde{\Theta}^S$ based on information theory, is not equivalent to previously defined similarity measures between partitions. Moreover the method is not affected significantly by the choice we made for treating inactive nodes or nodes belonging to connected components of two nodes. Although it might be a challenging technical problem to assess which of the similarity measures proposed so far is the best, the similarity measure $\tilde{\Theta}^S$ seems to be more relevant of other similarity measures used in the literature when applied to the APS Collaboration Multiplex Networks. In fact the partition obtained by using the similarity measure $\tilde{\Theta}^S$ reflect much more closely the general perception of the organization of collaborations in the physics community.

VI. CONCLUSIONS

Characterizing the mesoscopic structure of multiplex networks is crucial to characterize large network datasets where the nodes are connected by different types of interactions. Such multilayer networks are ubiquitous, and systems as different as social networks, transportation networks or cellular and brain networks require a multilayer description. Here, by using information theory tools, we have defined an indicator function $\tilde{\Theta}^S$ able to measure the mesoscopic similarities between the layers of a multiplex network. This indicator can be used to quantitatively compare the layers of a multiplex network with respect to the mesoscopic structure induced by any feature depending on the layer architecture. In particular here we have focused on the case in which the feature of the nodes is their community assignment. We have shown that $\tilde{\Theta}^S$ can reveal the network between the layers of a multiplex and we have applied this method to the Collaboration Multiplex Network at the two levels of the PACS hierarchy, obtaining a bottom-up approach to identify how the organization of knowledge in physics is reflected in the structure of collaboration networks.

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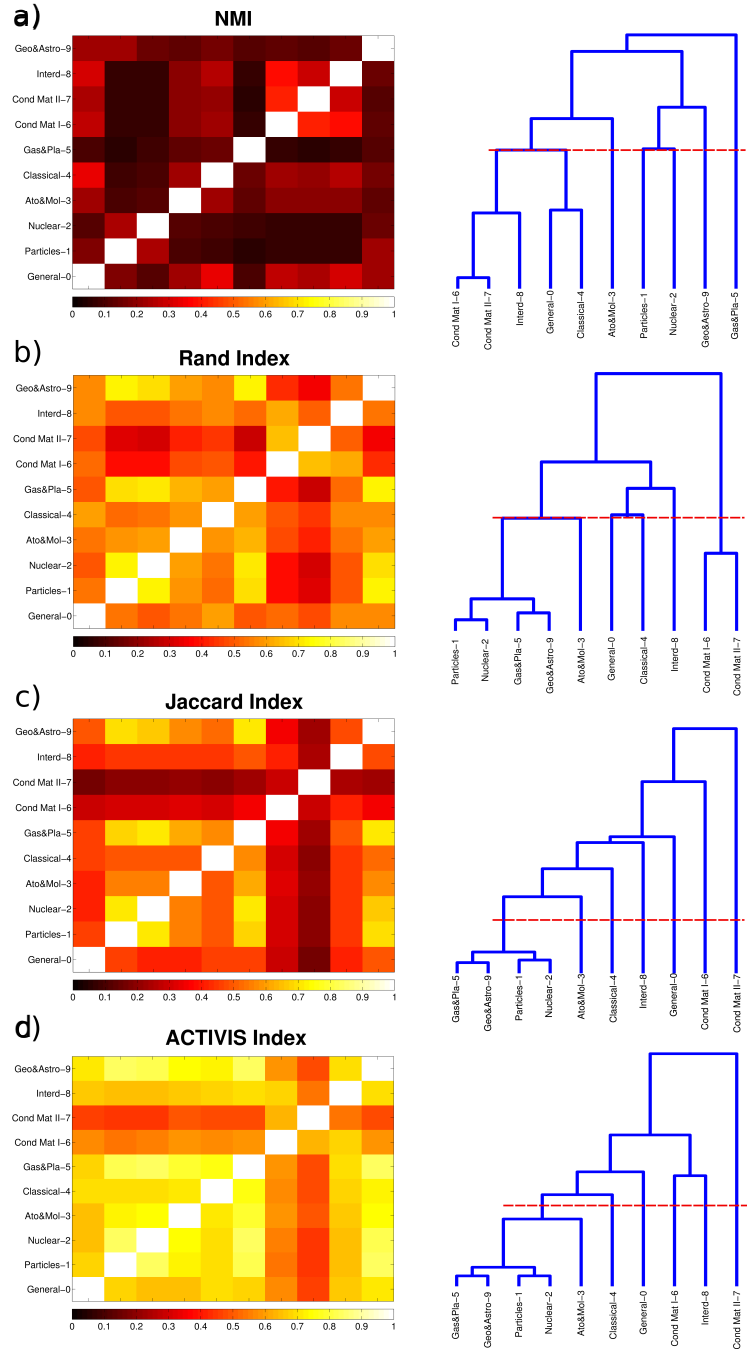


FIG. 9: (Color online) Other similarity measures used to hierarchically cluster the $M_1 = 10$ layers of the APS Collaboration Multiplex Network at the first level of the PACS hierarchy. The similarity matrices and their respective dendrograms cutted at the partition optimizing the modularity Q (red-dashed line) are shown for the Normalized Mutual Information (Panel a), Rand Index (Panel b), Jaccard Index (Panel c) and for the *ACTIVIS* Index (Panel d). Layer partitions are obtained using the Infomap community detection algorithm. None of the optimal partitions corresponds to the one obtained using $\tilde{\Theta}^S$ to measure similarities.

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